Cyclobutanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester
160790-09-0 | DTXSID20166995

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.91e-04 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.90e-01

Confidence level: 3.93e-01

Nearest Neighbors from the Training Set

Image not found

Endosulfan sulfate

Measured: 1.14e-06

Predicted: 6.86e-06

Image not found

Cyclopropanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, methyl ester

Measured: 4.91e-04

Predicted: 9.14e-04

Image not found

Cyclobutanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester

Measured: 1.00e-03

Predicted: 3.91e-04

Image not found

Oxycarboxin

Measured: 4.43e-03

Predicted: 8.70e-04